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Four fully configured and networked IBM/RISK 6000 3BT work stations/ with peripherals have been purchased for performing high level ab initio calculations on high energy compounds

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COMPUTATIONS ON HIGH ENERGY COMPOUNDS
— AN INSTRUMENTATION REQUEST —

This final report describes the computer equipment, peripherals, and software purchased to conduct computations on high energy compounds. A synopsis of the intended use is also provided.

I. PURCHASE OF THE INSTRUMENTATION

The hardware configuration was chosen after two rounds of requests for proposals from vendors of workstations and disk drives. The printer and software were obtained from designated vendors. The rapid advancements in c.p.u. and disk drive technology enabled the purchase of significantly faster and more complete workstations than those formulated in the grant proposal. Computer workstation from IBM, Hewlett Packard, Silicon Graphics, and Kubota (DEC) were considered. The following equipment and software has been purchased:

Vendor: IBM - Birmingham, AL

1 IBM RISC/6000 Model 3BT Server
This system contains 128 Mb, 2 Gb disk, 0.5 Mb cache, CD-ROM, 4.0 Gb 4 mm tape, 3.5" diskette, 20" color monitor, power GT4E graphics adapter, SCSI-2 adapter, AIX 3.2.5, AIX Windows, Fortran V3.

3 IBM RISC/6000 Model 3BT
This system contains 128 Mb, 2 Gb disk, 3.5" diskette, 20" color monitor, power GT4E graphics adapter, SCSI-2 adapter, AIX 3.2.5, AIX Windows, Fortran V2.

Total IBM Configuration Price $ 130,000

Vendor: Western Scientific - Evergreen, CO

1 Toolbox with 3 IBM 2Gb SCSI-2 disk drives

3 Toolbox with 2 IBM 2Gb SCSI-2 disk drives

Total Western Scientific Price $ 15,530

Vendor: Middle South Computers - Jackson, MS

1 HP Laser Jet 4SiMX
This is a network HP and Postscript printer, 17 pages/min, 10 Mb.

Total Middle South Computers Price $ 3,758

Vendor: Wave Function, Inc - Irvine, CA

3 SPARTAN 3.1
Quantum Chemistry Visualization software, 3 licenses

Total Wave Function, Inc Price $ 2,250

Total all purchases $ 151,538

This grant provided for $ 100,000 toward the $ 151,538 for the purchase of the listed equipment. UAB provided $ 51,538 in matching moneys toward the purchase of the equipment and software.

The purchased equipment exceeds in c.p.u. performance, memory, graphics, disk space, configuration, and balance both the IBM and Kubota (DEC) quotes formulated in the awarded grant. Specifications of the c.p.u. are listed below with those of the IBM/RISK600 580, 375, and the DEC 500 and 400 workstations that were listed in the proposal. The LINPACK specs for the IBM 3BT are 55.1 (100x100) and 183 (1000x1000).

workstation	SPECfp92	SPECint92
IBM 3BT	205.3	114.0
IBM 580	133.2	67.1
DEC 500	126.0	74.3
IBM 375	118.2	59.8
DEC 400	112.2	65.3

The following software will be added to the system, but its intended purchase with UAB funds was postponed in order to obtain the latest, delayed release of Gaussian 94.

Vendor: Gaussian, Inc - Pittsburgh, PA

1 Upgrade of GAUSSIAN 92 to GAUSSIAN 94
Quantum Chemistry software, license upgrade

Total Gaussian Inc Price $ 1,001

The above listed equipment has replaced (a) a cluster of networked VAXes (1 μVAX, 2 VAXstations 3200, and 2 VAXstations 2000), (b) a Stardent 3010 (Titan), which was loaned by Kubota Pacific Computer Inc. to Lammertsma for 1991 and 1992, and (c) will soon replace the remaining dated Stardent 3020 (Titan, purchased in 1989), which is, however, still performing and being serviced.

II. INSTALLATION OF THE INSTRUMENTATION

The cluster of workstations and the printer were installed and networked in the summer of 1994, with three of the workstations arriving in late June and the server in August, 1994. The server upgrade with L2 cache occurred in November. OpenGL shipped in late August, and missing prerequisites were received in December. Quantum chemistry software was ported from the existing cluster of workstations to the IBM cluster. The ported software includes GAUSSIAN 92, PSI 2.0, and ACES, all of which has been verified to run under the NFS protocol on the new equipment. SPARTAN 3.1 has been installed. Graphics manipulations were required to bring about a seamless transfer of data between the IBM cluster and the Stardent 3020.

III. USE OF THE INSTRUMENTATION

The instrumentation forms the backbone of the AFOSR grant awarded to Lammertsma, entitled "Insensitive High Explosives — A Computational Study," (FQ8671-9401529), which had a starting date of September 31, 1994. The equipment is used by Hamilton to investigate the novel use of scaled hermite gaussian functions (HGFs) in derivative codes.

Insensitive High Explosives – This work is a natural extension to our earlier study on the tautomeric processes that may underlie the sensitivities of picric acid, picramide, and TNT. We reported this in Final Report WL-TR-93-7062, entitled "On the viability of nitronic acids in the decomposition of nitroaromatics – A theoretical study of nitronic acids." The current computations involve tautomeric studies to complement those of nitromethane, acetaldehyde, and acetimine. Studies have begun to quantify the tautomeric processes in nitramine, methylnitramine, formaldehyde, nitrosomethane, and imidoxime. These computations are directed toward addressing the stabilities of the explosives 3-nitro-1,2,4-triazole-5-one (NTO), hexahydro-1-nitro-1,3,5-triazine, and hexahydro-1,3-dinitro- and 1,3,5-trinitrotriazine (RDX) using high level *ab initio* theory. In these studies rearrangements and possible dissociation pathways are mapped using Bader's electron density analysis. Additional porting of graphics software to the IBM cluster may be required for visualization of these analyses. Solvation effects on the tautomeric equilibria will be evaluated with GAUSSIAN 94 which should enable a more reliable analysis than hitherto feasible. Excitation energies will also be determined with this suite of programs. With the additional PSI 2.0 and ACES codes we are now better equipped to determine accurate bond dissociations. Work is in progress on the parent tautomeric processes. A graduate student has been attracted in the past quarter for this research and a postdoctoral fellow has been identified and is to arrive shortly.

In addition the workstations will be used to continue our computational work on small binary clusters. Particularly, emphasis will be placed on exploring the structures and energies of Li/B and Li/Al combinations and their hydrogenated derivatives.

Scaled hermite gaussian functions – A pilot code is being written using the recursive Rys polynomial method for the construction of the derivative two-electron repulsion integrals (ij|kl). The construction of the intermediates for centers i and k are much the same, with only slight modification of the coefficients used in the recurrence relations. The buildup of angular momentum on centers j and l leads to more complicated equations than the transfer relations needed for Cartesian gaussians.

During the course of the above research, the use of rotational invariance in two-electron integral derivatives was reconsidered. No derivative codes currently use this property because of the logic involved (accounting for exceptions due to redundancy and/or collinearity and/or coplanarity of centers). We are applying rotational invariance to the forces generated after contraction of the density factors with the integral derivatives, producing fewer linear equations to solve. Additionally, the rotational invariance equations need to be solved much fewer times if *all* of the contributions to the forces are added together for a particular choice of four nuclei.

The preliminary work is described in an abstract to the Sanibel Symposium and will be submitted to the symposium issue of the International Journal of Quantum Chemistry.